

ABSTRACT

5           The present invention relates to a data storage  
medium encoded with the corresponding structure  
coordinates of molecules and molecular complexes which  
comprise the active site binding pockets of JNK3. A  
computer comprising such data storage material is capable  
10 of displaying such molecules and molecular complexes, or  
their structural homologues, as a graphical three-  
dimensional representation on a computer screen. This  
invention also relates to methods of using the structure  
coordinates to solve the structure of homologous proteins  
15 or protein complexes. In addition, this invention  
relates to methods of using the structure coordinates to  
screen and design compounds, including inhibitory  
compounds, that bind to JNK3 or homologues thereof. This  
invention also relates to molecules and molecular  
20 complexes which comprise the active site binding pockets  
of JNK3 or close structural homologues of the active site  
binding pockets.